Collection des données: *CAD-4-Express* (Duisenberg, 1992; Macíček & Yordanov, 1992). Affinement des paramètres de la maille: *CAD-4-Express*. Réduction des données: *MolEN* (Fair, 1990). Programme(s) pour la solution de la structure: *SHELXS86* (Sheldrick, 1990). Programme(s) pour l'affinement de la structure: *SHELXL93* (Sheldrick, 1993). Logiciel utilisé pour préparer le matériel pour publication: *SHELXL93*.

Les listes des facteurs d'agitation thermique et des facteurs de structure ont été déposées au dépôt d'archives de l'UICr (Référence: DU1161). On peut en obtenir des copies en s'adressant à: The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

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Strontium Metagermanate, $SrGeO_3$

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Abstract

This form of strontium germanium trioxide has the same structure as that reported by Hilmer [*Sov. Phys. Crystallogr.* (1963), **7**(5), 573–576] except that it has monoclinic rather than hexagonal symmetry. Two forms of $SrGeO_3$ are known at present: this monoclinic form and a triclinic form reported by Nadezhina, Pobedimskaya, Ilyukhin & Belov [*Sov. Phys. Crystallogr.* (1981), **26**(1), 27–32; **26**(3), 268–271]. The present structure has alternate stacking of ternary rings of GeO_4 groups and close-packed Sr atoms along [001], and is a six-layer polytype.

Comment

$SrGeO_3$ has been studied previously by one person and one group. Hilmer (1963) studied the crystal structure of $SrGeO_3$ using a Weissenberg camera. He obtained hexagonal lattice parameters (a = 7.29, c = 31.64 Å) and showed that the structure contained ternary rings of GeO_4 groups. In addition, he concluded that the structure was composed of alternating layers of $[Ge_3O_9]^{6-}$ rings and layers of Sr atoms. Nadezhina, Pobedimskaya, Ilyukhin & Belov (1981*a*,*b*) also studied $SrGeO_3$ but obtained triclinic lattice parameters (a = 8.699, b = 9.935, c = 11.148 Å, α = 106.04, β = 89.97, γ = 102.11°). This structure also contained rings of GeO_4 groups, but the configurations of the rings were quite different from those in the structure described by Hilmer (1963). Nadezhina *et al.* (1981*a*,*b*) stated that the different types of ternary rings in the two modifications of strontium metagermanate were undoubtedly the result of a difference in the structures of the cation layers. In addition, they called the form they had studied the low-temperature form (α'-$SrGeO_3$) and the form Hilmer had studied the high-temperature form (α-$SrGeO_3$). Yamanaka & Mori (1981) solved the structure of α-$CaSiO_3$ (pseudowollastonite) and found the structure to be characterized by four layers, each of which was composed of ternary rings of SiO_4 groups and a Ca polyhedron layer. They compared the structure of α-$CaSiO_3$ with the structure of $SrGeO_3$ determined by Hilmer and predicted that the latter contained six layers.

The symmetry and the lattice parameters of $SrGeO_3$ found in the present work are different not only from those given by Hilmer (1963) but also from those given by Nadezhina *et al.* (1981*a*,*b*). However, this structure is the same that described by Hilmer for two reasons. Firstly, the crystal studied here has a pseudo-hexagonal cell which corresponds to the cell given by Hilmer. Secondly, all of the reflections observed by Hilmer can be indexed on the basis of the present monoclinic cell and their intensities are very similar. The structure described by Nadezhina *et al.* is different, so two forms of $SrGeO_3$ exist.

Fig. 1 shows the arrangement of the ternary rings and the Sr atoms in the present structure. It is notable that the Sr atoms form a close-packed layer. Fig. 2 shows the layers of ternary rings of GeO_4 groups and the layers of Sr atoms stacked alternately along [001]. The unique edges of the GeO_4 tetrahedra are almost parallel to the stacking direction. Yamanaka & Mori (1981) defined a layer as one layer of the ternary rings plus one layer of Sr atoms. In the present structure the seventh layer is located just above the first layer along the stacking direction, suggesting that this is a six-layer structure. The mean values of the Sr(1)—O and

Sr(2)—O bond lengths are 2.667 (2) and 2.678 (2) Å, respectively (Table 2). These are significantly shorter than those in $SrGe_4O_9$ [2.760 (3) Å], which also contains ternary rings of GeO_4 groups (Nishi, 1996). The Ge—O—Ge angles in the ring are 132.0 (5) and 133.5 (3)° (Table 2). The corresponding angles in the structure described by Nadezhina *et al.* (1981*a*,*b*) range from 118.3 to 121.2° and those in $SrGe_4O_9$ (Nishi, 1996) are 121.2 (4) and 123.8 (5)°. The values in the present structure are distinctly larger and are similar to those in α-$CaSiO_3$ (134.5–135.6°; Yamanaka & Mori, 1981), suggesting that the two structures contain the same kind of ternary rings.

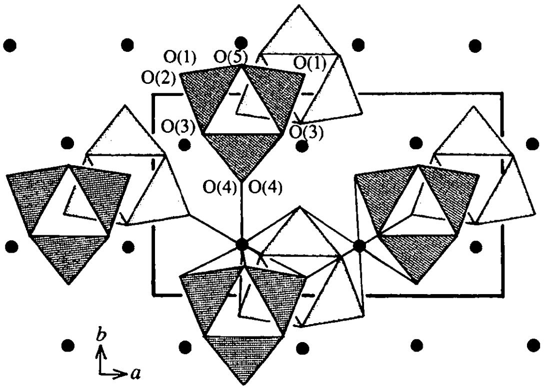

Fig. 1. The $SrGeO_3$ structure viewed along [001] showing the arrangement of the Ge_3O_9 rings at $z \simeq 3/4$ (dark rings) and those at $z \simeq 1/4$ (light rings). The solid circles represent Sr atoms at $z \simeq 1/2$.

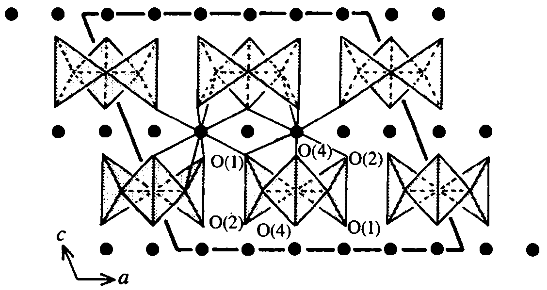

Fig. 2. The $SrGeO_3$ structure viewed down the *b* axis showing the arrangement of the layers of Ge_3O_9 rings and SrO_8 polyhedra. The solid circles represent Sr atoms.

Experimental

Single crystals of strontium metagermanate were synthesized from a stoichiometric mixture of $SrCl_2$ and GeO_2 at 1570 K. Electron microprobe analyses of the crystals showed that they had the chemical formula $SrGeO_3$. The intensities of the reflections were measured at the X-ray Laboratory of Nihon University, Japan.

Crystal data

$SrGeO_3$
$M_r = 208.21$
Monoclinic
$C2/c$
$a = 12.533 (3)$ Å
$b = 7.262 (1)$ Å
$c = 11.259 (3)$ Å
$\beta = 111.30 (2)°$
$V = 954.7 (4)$ Å^3
$Z = 12$
$D_x = 4.35$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 24 reflections
$\theta = 19.8$–$35.8°$
$\mu = 27.31$ mm^{-1}
$T = 293$ K
Sphere
0.14 mm (radius)
Colourless

Data collection

Rigaku AFC-5 diffractometer
$\omega/2\theta$ scans
Absorption correction: spherical
$T_{min} = 0.117$, $T_{max} = 0.157$
4619 measured reflections
1529 independent reflections
1356 reflections with $I > 3\sigma(I)$

$R_{int} = 0.046$
$\theta_{max} = 35°$
$h = -19 \rightarrow 17$
$k = -10 \rightarrow 10$
$l = 0 \rightarrow 18$
3 standard reflections every 150 reflections intensity decay: 0.5%

Refinement

Refinement on F
$R = 0.048$
$wR = 0.033$
$S = 1.37$
1356 reflections
72 parameters
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} = 0.06$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Extinction correction: isotropic (Zachariasen, 1963)
Extinction coefficient: 3.79×10^{-6}
Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Sr(1)	0.08596 (8)	0.24326 (14)	0.49931 (10)	0.0101 (3)
Sr(2)	1/4	1/4	0	0.0107 (3)
Ge(1)	0.12921 (8)	0.45256 (13)	0.24627 (9)	0.0082 (2)
Ge(2)	0	0.84276 (19)	1/4	0.0086 (3)
O(1)	0.1262 (5)	0.4063 (8)	0.0959 (6)	0.011 (1)
O(2)	0.2273 (5)	0.4022 (9)	0.3927 (6)	0.016 (2)
O(3)	0.1130 (5)	0.6965 (7)	0.2483 (6)	0.013 (2)
O(4)	0.0503 (5)	0.9394 (9)	0.3969 (6)	0.013 (2)
O(5)	0	0.3523 (12)	1/4	0.014 (2)

Table 2. *Selected geometric parameters (Å, °)*

Sr(1)—O(2^{i})	2.451 (6)	Sr(2)—O(3^{vii})	2.756 (6)
Sr(1)—O(4^{ii})	2.454 (6)	Sr(2)—O(3^{viii})	2.756 (6)
Sr(1)—O(2)	2.730 (6)	Sr(2)—O(2^{vii})	2.770 (6)

Sr(1)—O(5)	2.733 (3)	Sr(2)—O($2^{\rm viii}$)	2.770 (6)
Sr(1)—O($3^{\rm iii}$)	2.734 (7)	Ge(1)—O(2)	1.700 (6)
Sr(1)—O($4^{\rm iv}$)	2.737 (6)	Ge(1)—O(1)	1.713 (6)
Sr(1)—O($1^{\rm iii}$)	2.741 (6)	Ge(1)—O(3)	1.784 (5)
Sr(1)—O($1^{\rm v}$)	2.748 (7)	Ge(1)—O(5)	1.790 (4)
Sr(2)—O(1)	2.466 (6)	Ge(2)—O(4)	1.694 (6)
Sr(2)—O($1^{\rm vi}$)	2.466 (6)	Ge(2)—O($4^{\rm v}$)	1.694 (6)
Sr(2)—O($4^{\rm vii}$)	2.719 (6)	Ge(2)—O(3)	1.776 (5)
Sr(2)—O($4^{\rm viii}$)	2.719 (6)	Ge(2)—O($3^{\rm v}$)	1.776 (5)
O(2)—Ge(1)—O(1)	131.7 (3)	O(4)—Ge(2)—O(3)	104.1 (3)
O(2)—Ge(1)—O(3)	104.3 (3)	O(4)—Ge(2)—O($3^{\rm v}$)	104.6 (3)
O(2)—Ge(1)—O(5)	103.4 (2)	O($4^{\rm v}$)—Ge(2)—O(3)	104.6 (3)
O(1)—Ge(1)—O(3)	104.2 (3)	O($4^{\rm v}$)—Ge(2)—O($3^{\rm v}$)	104.1 (3)
O(1)—Ge(1)—O(5)	104.4 (2)	O(3)—Ge(2)—O($3^{\rm v}$)	106.5 (3)
O(3)—Ge(1)—O(5)	107.2 (3)	Ge(2)—O(3)—Ge(1)	133.5 (3)
O(4)—Ge(2)—O($4^{\rm v}$)	131.0 (3)	Ge(1)—O(5)—Ge($1^{\rm v}$)	132.0 (5)

Symmetry codes: (i) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$; (ii) $x, y-1, z$; (iii) $x, 1-y, \frac{1}{2}+z$; (iv) $-x, 1-y, 1-z$; (v) $-x, y, \frac{1}{2}-z$; (vi) $\frac{1}{2}-x, \frac{1}{2}-y, -z$; (vii) $x, 1-y, z-\frac{1}{2}$; (viii) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$.

Data collection and cell refinement: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992*a*). Data reduction: *TEXSAN* (Molecular Structure Corporation, 1992*b*). Program(s) used to solve and refine structure: *LINUS* (Coppens & Hamilton, 1970). Program(s) used to calculate Fourier maps: *ORFFE* (Busing, Martin & Levy, 1964).

Lists of displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: BR1159). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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